Electronic Structure of Quasicrystals

Band Structure Is Similar to That of Normal Metals

Weirdness. It's the stock in trade of those uncannily regular yet aperiodic alloys known as quasicrystals. Though these materials' intriguing atomic structures have been closely scrutinized, scientists have only recently taken a solid step toward directly probing their electronic structure. In work carried out at Beamline 7.0.1, an international group of researchers has discovered that the electrons in quasicrystals behave surprisingly like electrons in normal metals. This development runs counter to the most promising theories of how electrons should move in these unpredictable alloys.

Atoms in a quasicrystal, like those in a more familiar crystal, have perfect long-range order. The twist is that the order is not based on a repeating unit cell but on a regular, predictable series of a different type. A one-dimensional analogy can be found in the Fibonacci sequence, where each value is the sum of the two previous values. The resulting series is regular but not periodic. Such rules of order generate crystals with rotational symmetries that, were the crystals periodic, would not not allow their unit cells to fill space without overlapping. In spite of the lack of periodicity, these crystals have perfectly sharp diffraction patterns that are as crisp as those imaged for the best ordinary, periodic crystals. In addition to their bizarre geometries, quasicrystals have counterintuitive properties. For example, though composed of elements that are good conductors in their pure form, they are themselves poor conductors that conduct more poorly as the lattice becomes more perfect. At low temperatures, they have magnetoresistances similar to those observed in giant magnetoresistive materials. Potentially useful properties include durability, stability, low stickiness, and the ability to store hydrogen at high density.

The ALS studies were performed on an AlNiCo alloy ($Al_{71.8}Ni_{14.8}Co_{13.4}$), a member of the decagonal family of quasicrystals, which is aperiodic in two dimensions and periodic in the third. These crystals have ten-fold symmetry in the aperiodic plane. The researchers analyzed the crystals by acquiring a series of angle-resolved photoemission spectra at the Ultra-ESCA endstation. These spectra collectively form an energy-momentum map that looks strikingly like the electronic bandmap of a conventional crystal.

The researchers found several intriguing aspects of the AlNiCo quasicrystals. They were able to track a single electronic state in both the aperiodic and periodic directions, showing that the same electronic state in the quasicrystal displayed both periodic and aperiodic character. They also noted three important similarities to the band structure of ordinary metals: Their work shows clear evidence of delocalized states (i.e., the electrons are not all confined to localized groups that move around a small cluster of atomic nuclei, as was predicted). The electrons also have an effective mass (a measure of how difficult it is for an electron to move through the crystal) comparable to a free electron's mass, rather than the nearly infinite mass predicted for quasicrystals. Finally, the researchers observed that the Fermi surface (a mapping of the allowed momenta of the least bound electrons) of a quasicrystal consists of well-defined contours. The topology of the Fermi surface should determine the electron transport properties of the material. That these features are related to the aperiodic order is evidenced by the fact that the band structure reflected the ten-fold structure of the aperiodic crystal plane. These new findings begin to answer the much-asked question of how electrons in quasicrystals move. The study clearly showed that they behave much more like those in ordinary metals than previously thought. ■

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E. Rotenberg, W. Theis, K. Horn, and P.Gille, "Quasicrystalline valence bands in decagonal AlNiCo," *Nature* **406**, 602 (2000).

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ELECTRONIC STRUCTURE OF QUASICRYSTALS

Band Structure Is Similar to That of Normal Metals

- **Quasicrystals are a class of materials with unusual properties**
  - *Aperiodic structure*
  - *Anomalous transport properties*
  - *Durability, stability, low stickiness, dense hydrogen storage*
- **AlNiCo alloy: quasicrystals with periodic stacking of 2-dimensional aperiodic planes**
- **Photoemission studies reveal electronic structure similar to that of a normal metal**
  - *Delocalized electron states*
  - *Effective mass of electrons similar to that of a free electron*
  - *Well-defined Fermi surface in both periodic and aperiodic directions*

E. Rotenberg (Lawrence Berkeley National Laboratory), W. Theis (Free University of Berlin), K. Horn (Fritz-Haber Institute, Berlin), and P.Gille (Ludwig-Maximilians University, Munich. [*Nature* **406**, 602 (2000)]

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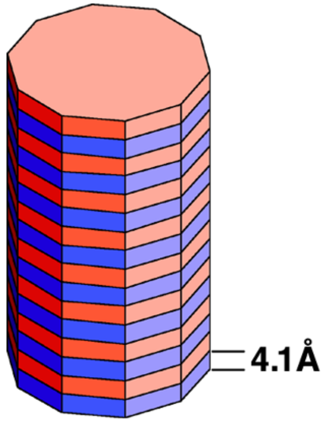
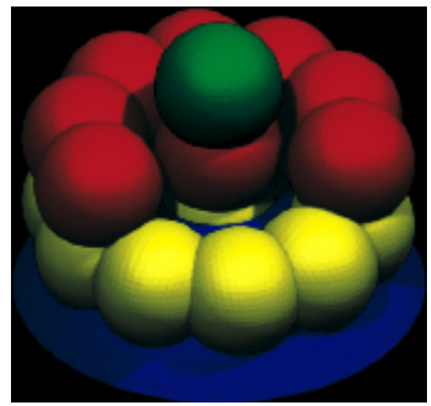


AlNiCo alloy has aperiodic order in two dimensions (axes parallel to the surface studied) and periodic order in the third. The aperiodic plane has ten-fold rotational symmetry.



Photoemission data (left) showed that the material contains nearly free electrons confined to spheres in momentum space. The model (right) based on that data shows that these spheres are arranged in 10-fold rings that are stacked periodically, reflecting the mixed periodic/aperiodic quasicrystalline character.

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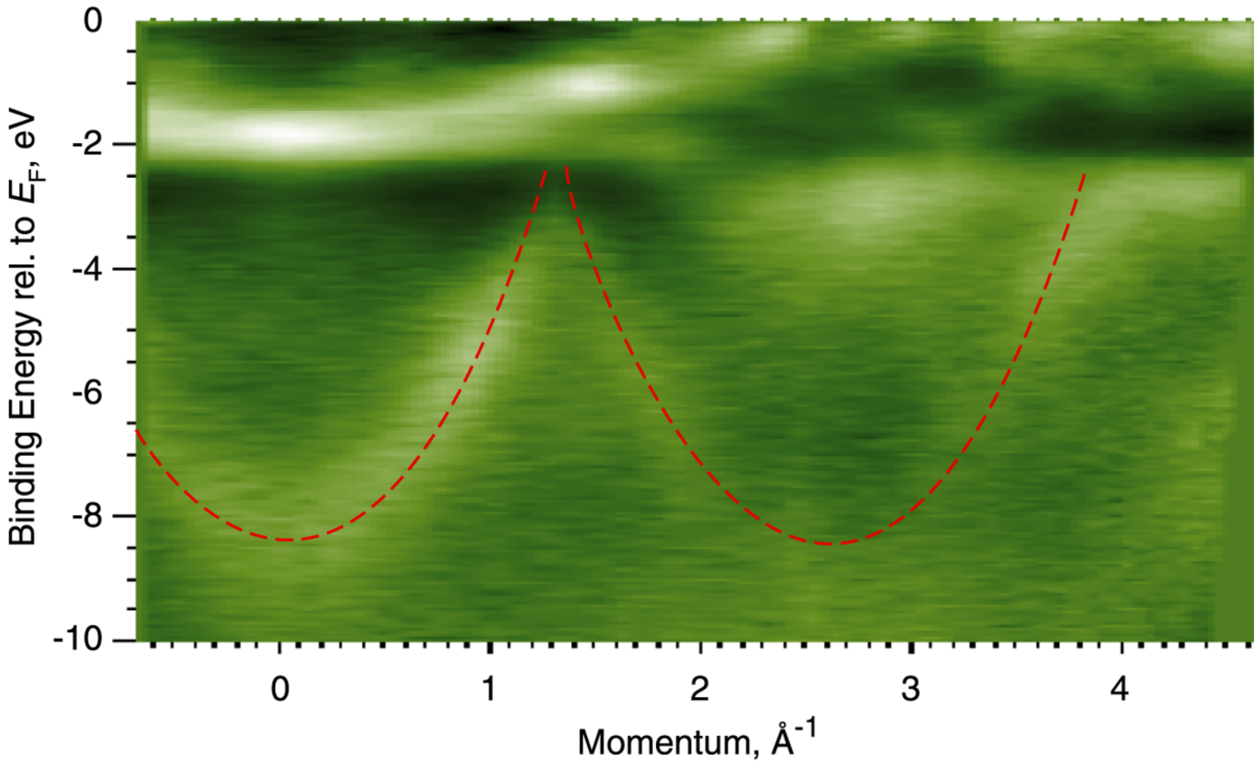

Collecting valence band spectra as a function of electron momentum in the aperiodic plane reveals features that are very similar to those seen in the band structures of ordinary periodic metals: a set of shallow d bands, some of which clearly cross the Fermi level, and a pair of deeper, parabolic s-p bands (dashed lines) with free-electron-like character. These give strong evidence for the existence of delocalized states in quasicrystals.

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